Topology Atlas Invited Contributions **9** (2004) no. 1, 12 pp.

COMPUTATIONAL TOPOLOGY FOR REGULAR CLOSED SETS (WITHIN THE I-TANGO PROJECT)

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Abstract. The Boolean algebra of regular closed sets is prominent in topology, particularly as a dual for the Stone-Čech compactification. This algebra is also central for the theory of geometric computation, as a representation for combinatorial operations on geometric sets. However, the issue of computational approximation introduces unresolved subtleties that do not occur within "pure" topology. One major effort towards reconciling this mathematical theory with computational practice is our ongoing I-TANGO project. The acronym I-TANGO is an abbreviation for "Intersections—Topology, Accuracy and Numerics for Geometric Objects". The long-range goals and initial progress of the I-TANGO team in development of computational topology are presented.

1. Introduction and brief literature review

Throughout this paper, all sets considered will be assumed to be subsets of $\mathbb{R}^3$, with its usual topology. The Boolean algebra of regular closed sets in $\mathbb{R}^3$ will be denoted as $\mathcal{R}(\mathbb{R}^3)$. Furthermore, any regular closed set considered will be assumed to be compact. Any surfaces and curves considered will be assumed to be compact 2-manifolds and 1-manifolds, respectively. All neighborhoods will be assumed to be open subsets of $\mathbb{R}^3$.

The theoretical role for $\mathcal{R}(\mathbb{R}^3)$ was introduced into geometric computing to correct the unexpected output seen from combinatorial operations on geometric sets [27]. For instance, consider the two dimensional illustration shown in Figure 1. The original operands of A and B are indicated in Figure 1(a). The unexpected output is shown in Figure 1(b), where the expected result would have been what is shown in Figure 1(c).

The phenomenon shown in Figure 1(b) was informally described as "dangling edges" [33]. The formalism that was proposed to eliminate this behavior was that geometric combinatorial algorithms should accept only regular closed sets as input and then execute the Boolean operations of meet, join and complementation on these operands, thereby creating only regular closed sets as output [32]. The intent

Date: November 2003.

Partial funding for all authors was from NSF grant DMS-0138098. Authors Peters and Sakkalis were also partially supported by NSF grant CCR 0226504. All statements in this publication are the responsibility of the authors, *not* of any of these indicated funding sources.

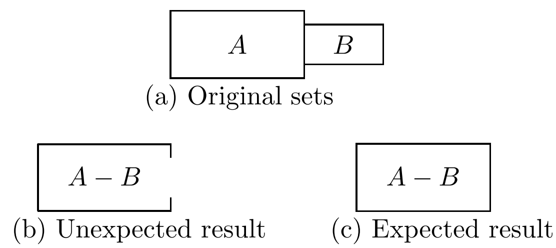

Figure 1. Subtraction of two sets

was to eliminate "dangling edges" and, in principle, this should have been sufficient[1]. However, each operand also has a geometric representation that depends upon the approximation methods used to compute the results. This additional subtlety raises issues in both theory and computation.

For this short article, only a brief literature review will be presented. An earlier survey on topology in computer-aided geometric design [25] is recommended as introductory material for topologists. The texts [15, 24] discuss the integration of computational geometry, shape modeling and topology. The subject of computational topology is still a nascent and emerging sub-discipline. This article focuses upon the authors' particular perspective in its development. The first use of the terminology "computational topology" appears to have been in the dissertation of M. Mäntylä [20]. Further contemporary views can be gained from the following web sites [6, 9, 34].

Additional perspective can be gained by understanding the broader context in which topology has already been successfully applied to computer science. We mention two particularly notable successes. The first is the use of non-Hausdorff topology by Kopperman, Meyer, Kong, Rosenfeld, Smyth and Herman in digital topology for computer graphics and image processing. A good overview is readily available [18]. Similarly, the work of Mislove, Reed and Roscoe on domains explores variants of limits for fundamental algorithmic and programming language studies, continuing the expressive power and the broad applicability of the language of topology in denotational semantics and concurrent programming. The monograph [26] is recommended as an introduction.

2. Theory versus computation

One elegant computational representation for the combinatorial operators is to assign each object a symbol and then to indicate operations in a tree referencing those symbols. For instance, such a tree structure could be as depicted in Figure 2.

At this level of abstraction, the mathematical theory and the computational representation are completely consistent, and this representation became known as Constructive Solid Geometry (CSG). Difficulties arose in instantiating the basic geometric information that is represented by the operands at the leaf nodes and, sometimes, in computing geometric representations at the internal nodes of the

[1]The subtraction operation between two sets, shown as $A - B$ in Figure 1, is not *specifically* a Boolean operation. However, the use of $A - B$ should be understood to be conveniently shortened notation equivalent to the operations $A \wedge B'$, where B' represents the standard Boolean operation of complementation on the operand B.

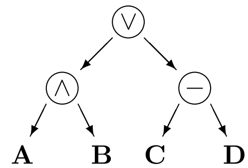

FIGURE 2. Tree for $(\mathbf{A} \wedge \mathbf{B}) \vee (\mathbf{C} - \mathbf{D})$.

tree. In CSG, the leaf nodes are restricted to a small set of specific geometric objects, known as primitives. A typical collection of primitives might consist of spheres, parallelepipeds, tori and right circular cylinders. The critical geometric algorithm underlying each Boolean operation is the pairwise intersection between the operands.

As the boundary of each of these primitives can be represented by linear or quadratic polynomials, the needed intersection between each pair of primitives was relatively simple and numerically stable, for most cases considered, although specific intersections could be problematical. For instance, suppose two cylinders of identical radius and height were created and then positioned so that the bottom of one cylinder was co-incident with the top of the other cylinder. This special case was specifically considered in most intersection algorithms and could usually be processed without problem. However, if one then rotated the top cylinder a fraction of a degree about its axis (so that the planar co-incidence remained intact) many software systems would fail to produce any output for this problem, sometimes even causing a catastrophic program failure. This particular problem became a celebrated test case and most systems developed *ad hoc* methods to solve this cylindrical intersection problem. Yet, this was just avoiding the more serious issue of the fragile theoretical foundations for many intersection algorithms. People using CSG systems became sensitive to their limitations and continued to use them effectively by avoiding these challenging circumstances, although the work-arounds were often tedious to execute.

The imperative, largely initiated by the aerospace and automotive industries, to model objects using polynomials of much higher degree than quadratic created a movement away from CSG systems. The alternative format was to represent compact elements of $\mathcal{R}(\mathbb{R}^3)$ by their boundaries, and this became known as the "boundary representation" approach, or "B-rep" for short. This has become the dominant mode today. Again, within this clean conceptual overview, the realities of computation pose some subtle problems. In most industrial practice, the modeling paradigm was further restricted so that the boundary of an object was a 2-manifold without boundary. However, it was difficult to create computer modeling tools that could globally define 2-manifolds without boundary, though there existed excellent tools for creating subsets of these 2-manifolds. For example, computational tools for creating splines were becoming prevalent. Again, in principle, if each such spline subset was created with its boundaries, then the subsets could be joined along shared boundary elements to form a topological complex [14] for the bounding 2-manifold without boundary.

The inherent computational difficulty was to separately create two spline patches, each being a manifold with boundary, so that the corresponding boundary curves

were identical and could be exactly shared between the patches. In some situations, algorithms for fitting spline patches were used successfully. In other cases, patches have been slightly enlarged and intersected so as to obtain improved fits. Indeed, such intersections are well-defined in pure mathematics, but, again, approximation in computation poses subtle variations from that theory, as described in the next section on pairwise surface intersection.

3. Subtleties of pairwise spline surface intersection

It is well-known that unwanted gaps between spline surfaces or self-intersections within intended manifolds often appear as unwanted artifacts of various implemented intersection algorithms [10]. The mismatch between approximate geometry and exact topology has historically caused reliability problems in graphics, CAD, and engineering analyses—drawing the attention of both academia and industry. The severity of the problem increases with the complexity of the geometric data represented, both from high-degree nonlinearity and from the intricate interdependence of shape elements that should, but do not, fit together according to the specified topological adjacency information.

The conceptual view of these joining operations is illustrated in Figure 3, with an intersection curve[2] denoted as c. But this picture of c only exemplifies the idealized, exact intersection curve. For practical computations, an approximation of c is often created [11] and, in many systems, an intersection curve will be approximated twice; once within the parametric domain of one of the intersecting surfaces and then again within the parametric domain of the other. These approximations are labeled as c_1 and c_2 in Figure 3. The spline functions from $[0, 1]^2$ into $\mathbb{R}^3$ then also rely upon algorithmic evaluation of these approximated intersection curves, as indicated by F and G in Figure 3. It is virtually certain that those evaluations will not be exactly equal in $\mathbb{R}^3$.

The mismatch between concept and reality depicted in Figure 3 creates ambiguity, as the intersection representation is sometimes considered as a unique set, from the symbolic topological view, and at other times as two approximating sets, from the geometric view.

4. Specific progress

To resolve this ambiguity, we are investigating richer representations. We introduce a neighborhood of the true, but unknown, intersection set. This neighborhood is created from newly determined rigorous upper bounds on the error incurred during efficient intersection approximations. To date, it has been convenient to create these neighborhoods as tubular neighborhoods [13], but broader generalizations seem to be possible.

The role of topological equivalence. Before introducing these bounding neighborhoods, we discuss the meaning of topological equivalence between an object and its approximations. We have proposed the use of ambient isotopy for this topological equivalence versus the more traditional equivalence by homeomorphism, as is explained more fully in our publications [2, 3, 4, 28, 29, 31]. Intuitively, two closed curves will not be ambient isotopic if they form different knots. Figure 4 shows

[2]We focus on the generic case of an intersection curve, although isolated points and co-incident areas can also arise, with similar complications.

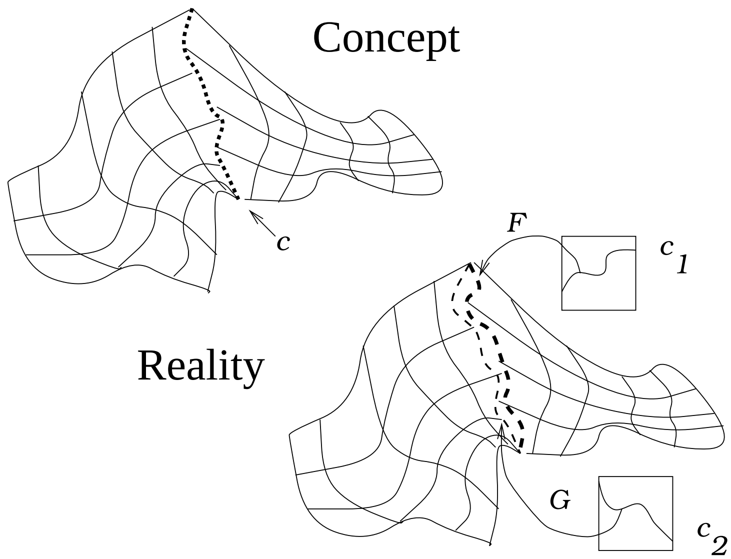

FIGURE 3. Joining operations for geometric objects

two simple homeomorphic space curves, where the piecewise linear (PL) curve is an approximation of the smooth curve. However, these curves are not ambient isotopic, because they depict different knots[3], with the smooth curve illustrating the simplest knot, known as the unknot. In the right half of Figure 4 the z coordinates of some vertices are specifically indicated to emphasize the knot crossings in $\mathbb{R}^3$ (All other end points have $z = 0$). All end points of the line segments in the PL approximation are also points on the original curve. Having this knotted curve as an approximant to the original unknot would be undesirable as output from a curve approximation algorithm, particularly for applications in graphics and engineering simulations. Similar pathologies can happen in approximating 2-manifolds, both with and without boundary, but results [2, 4, 19, 28, 29] summarized here can prevent these difficulties by appropriately constraining the approximations produced.

In response to the example of Figure 4, a theorem was published that provided for ambient isotopic PL approximations of 1-manifolds [19]. The proof utilizes "pipe surfaces" from classical differential geometry [21] to build an appropriately small tubular neighborhood such that if the PL approximant is constrained to lie within the constructed neighborhood, then the PL approximant is ambient isotopic to the original curve. While the techniques of tubular neighborhoods are well known in differential topology, the relevant theorems usually state only the existence of an ambient isotopy. Additional work in applied mathematics was needed to complement the theorems with constructive formulations from which to obtain effective procedures and algorithms. Such extensions were successfully accomplished for both non-singular compact, orientable 1-manifolds and 2-manifolds (with or without boundary) [1, 2, 19, 28, 29] by I-TANGO team members (and their co-authors). We used geometric characteristics to compute a *specific* upper bound on the size of a tubular neighborhood and to then specify a *particular* isotopy.

[3]The different knot classifications of 0_1 and 4_1^m are indicated in Figure 4.

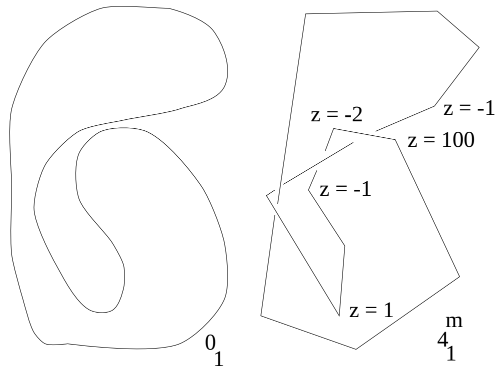

FIGURE 4. Nonequivalent knots

The importance of this topological equivalence class extends beyond the manifolds described to the geometric models created as compact subsets of $\mathcal{R}(\mathbb{R}^3)$. Consider that a well-defined topological complex could be created from 2-manifolds with boundary if the difficulties along the intersection boundaries could be solved. However, the non-uniqueness of the geometric representation of the intersection sets seems to pose an intractable problem to creation of a single, well-defined topological complex. Our alternative approach is to find a neighborhood within which it can be proven that the true intersection curve lies. Since the construction of these bounding neighborhoods is dependant upon the specific intersection algorithm used, some further details of the two intersection algorithms used within the I-TANGO project are presented. While the neighborhood construction details will vary with the specific intersection algorithm chosen, the following two neighborhood constructions were chosen both for their carefully defined error bounds and for their potential for generalization.

Error bounds for topology from Taylor's theorem. First, we present the Grandine-Klein (GK) intersection algorithm [12]. Referring to Figure 3, we note that the GK algorithm bases its error bounds on well-established numerical techniques in differential algebraic equations (DAE). While these DAE techniques provide rigorous error bounds, these bounds are expressed within the parameter space $[0,1]^2$, which serves as the domain of the spline functions (indicated as F and G in Figure 3). The code implementing the GK algorithm then has an interface that allows the user to specify an upper bound ϵ for this error in parameter space and the algorithm provides guarantees for meeting this error bound. However, the typical end user is often unaware of the role of this parametric domain, so selection of this parametric space error bound has often relied upon heuristics. It would be more convenient for the user to be able to specify an error bound within $\mathbb{R}^3$. One accomplishment within the I-TANGO project has been to demonstrate a mathematical relation [22] between the error bounds in $\mathbb{R}^3$ and $[0,1]^2$, following from a straightforward application of Taylor's Theorem in two dimensions [8, p. 200]. The conversion between these error bounds has been implemented in a pre-processing interface to the GK algorithm and this new interface has been tested to be reliable, efficient and user-friendly.

Using the notation from Figure 3 for the spline function F, Taylor's Theorem provides a bound on the error of F evaluated at a particular point (u, v) versus F evaluated at a point (u_0, v_0), where (u, v) and (u_0, v_0) are within a sufficiently small neighborhood. This sufficiently small neighborhood will have radius given by the value in the parametric domain $[0, 1]^2$ which was denoted as ϵ in the previous paragraph. Then it follows [22], with $\| \cdot \|$ being any convenient vector norm, that

$$\|F(u, v) - F(u_0, v_0)\| \le \epsilon M$$

for any M satisfying

$$\left\| \frac{\partial F}{\partial u}(u^*, v^*) \right\| + \left\| \frac{\partial F}{\partial v}(u^*, v^*) \right\| \le M,$$

for some point $[u^*, v^*]$ on the line segment joining $[u, v]$ and $[u_1, v_1]$.

For the single spline F, let $\gamma(F)$ be an upper bound for the acceptable error in $\mathbb{R}^3$ between the true intersection curve c and one of its approximants $F(c_1)$. In order to guarantee that this error is sufficiently small, it is sufficient

$$\epsilon M \le \gamma(F),$$

where an upper bound for M can be computed by using any standard technique for obtaining the maximums of the partials $\frac{\partial F}{\partial u}$ and $\frac{\partial F}{\partial v}$. For G, a similar relation between $\gamma(G)$ and ϵ exists[4].

Then it is clear that a neighborhood can be defined that contains the true intersection curve c and both of its approximants. Let $F(c_1)$ denote the image of c_1 under F and similarly, let $G(c_2)$ denote the image of c_2 under G. Let $N_{\gamma(F)}(F(c_1))$ be a tubular neighborhood of radius $\gamma(F)$ about $F(c_1)$, where c_1 has been generated from the GK intersector to satisfy the inequality presented in the previous paragraph. Similarly, define $N_{\gamma(G)}(G(c_2))$. Then, let

$$N(c) = N_{\gamma(F)}(F(c_1)) \cup N_{\gamma(G)}(G(c_2)).$$

It is clear that $N(c)$ is a neighborhood of c, which contains both of its approximants, $F(c_1)$ and $G(c_2)$. However, there is both a theoretical and computational limitation to this approach.

- There is no theoretical guarantee that either approximant is topologically equivalent to c, and
- Any practical computation of $N(c)$ would depend upon an accurate computation of the set $N_{\gamma(F)}(F(c_1)) \cap N_{\gamma(G)}(G(c_2))$, which is likely to be as difficult as the original computation of $F \cap G$.

While the above bounds are often quite acceptable in practice to compute a reasonable approximant, further research has been completed into alternate methods to give guarantees of topological equivalence within a computationally acceptable neighborhood of the intersection set, as reported in the next subsection.

Integrating error bounds and topology via interval solids. Recent work by Sakkalis, Shen and Patrikalakis [30] emphasized that the numeric input to any intersection algorithm has an initial approximation in the co-ordinates used to represent points in $\mathbb{R}^3$, leading to their use of interval arithmetic [24]. The basic idea behind interval arithmetic is that any operation on a real value v is replaced

[4]This error bound assumed that the error due to algorithmic truncation within the numerical DAE methods dominated any other computational errors.

by an operation of an interval of the form $[a, b]$, where $a, b \in \mathbb{R}$ and $a < v < b$. The result of any such interval operation is an interval, which is guaranteed to contain the true result of the operation on v. This led naturally to the concept of an *interval solid* and some of its fundamental topological and geometric properties were then proven, as summarized below.

Throughout this section, a *box* is a rectangular, closed parallelepiped in $\mathbb{R}^3$ with positive volume, whose edges are parallel to the co-ordinate axes[5]. Let F be a non-empty, compact, connected 2-manifold without boundary. Then the Jordan Surface Separation Theorem asserts that the complement of F in $\mathbb{R}^3$ has precisely two connected components, F_I, F_O; we may assume that F_I is bounded and F_O is unbounded. Let also $\mathcal{B} = \{b_j, j \in J\}$ be a finite collection of boxes that satisfies the following conditions:

- **C1:** $\{\mathrm{Int}(b_j), j \in J\}$ is a cover of F.
- **C2:** Each member b of $\mathcal{B}$ intersects F generically; that is, $b \cap F$ is a non-empty closed disk that separates b into two (closed) balls, B_b^+ and B_b^-, with B_b^+, (B_b^-) lying in $F_I \cup F$ ($F_O \cup F$), respectively.
- **C3:** For any $b_i, b_j \in \mathcal{B}$, let $b_{ij} = b_i \cap b_j$. If $\mathrm{Int}(b_i) \cap \mathrm{Int}(b_j) \neq \emptyset$, then b_{ij} is also a box which satisfies **C2**.

Notice that condition **C2** indicates that every $b \in \mathcal{B}$ intersects F in a natural way (see Figure 5).

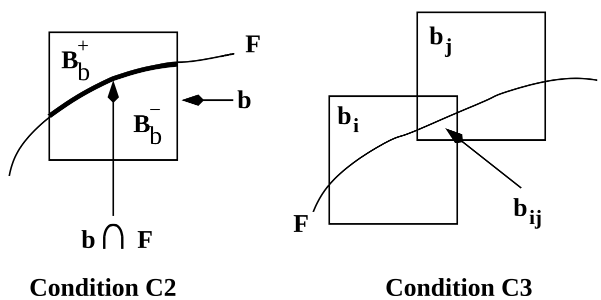

FIGURE 5. 2D versions of conditions **C2** and **C3**

The following result summarizes several previously appearing results, where a solid is defined to be a non-empty compact, regular closed subset of $\mathbb{R}^3$.

Theorem 4.1 ([30, Corollary 2.1, p. 165])**.** *If F is connected and $\mathcal{B}$ satisfies* **C1**–**C3***, then $F \cup \bigcup_{j \in J} b_j$ is a solid.*

Bisceglio, Peters and Sakkalis [28, 29] have recently given sufficient conditions to show when the boundary of an interval solid is ambient isotopic to the well-formed solid that it is approximating, as described in the following theorem. For a positive number δ, define the open set

$$F(\delta) = \{x \in \mathbb{R}^3 \mid D(x, F) < \delta\},$$

where $D(x, F) = \inf\{d(x, y) \mid y \in F\}$, with d being the usual Euclidean metric in $\mathbb{R}^3$.

[5]Enclosures other than boxes are quite possible and this is a subject of active research.

Theorem 4.2. *Let F be a connected 2-manifold without boundary. For each $\epsilon > 0$, there exists δ, with $0 < \delta < \rho$ so that whenever a family of boxes $\mathcal{B}$ satisfies conditions* **C1**–**C3**, *and for each b of $\mathcal{B}$, b is a subset of $F(\delta)$* (Please see Figure 6) *then, for $S = F \cup F_I$ and $S^{\mathcal{B}} = S \cup \bigcup_{j \in J} b_j$, the sets F and $\partial S^{\mathcal{B}}$ are ϵ-isotopic with compact support. Hence, they are also ambient isotopic.*

The quoted theorem depends upon results from Bing's book on PL topology [7, p. 214], and related literature [17], as is explained in full [28, 29]. The proof shows that normals to F do not intersect within the constructed tubular neighborhood, as is illustrated by the depiction of its planar cross-section in Figure 6.

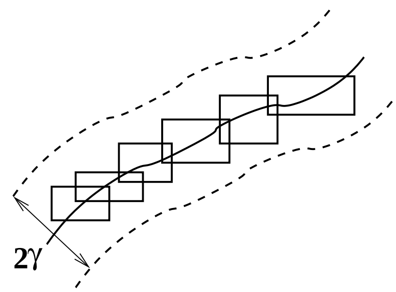

FIGURE 6. 2D version of proper subset condition

If the boxes containing the true intersection curve can be made sufficiently small so that each such box fits inside $F(\rho)$, then the resultant intersection neighborhood will contain an object that is both close to the true solid and is ambient isotopic to it. Considerable success in meeting these constraints has already been achieved [24] when two splines intersect transversally, while very recent progress from the I-TANGO team for more subtle spline intersection pairs is now under review [23]. As a further note on integration, results on root computations from interval arithmetic [24] are used to provide estimates of initial starting points for the GK algorithm.

Work in Progress. The previous discussion emphasizes results from the I-TANGO project that have already appeared in the literature, whereas the remarks in this section are intended to provide some indication of related results that are expected to appear soon.

Recall that the result of the GK algorithm will be a set of spline patches that do not fit together precisely along the approximation of their boundary. Recent work by Andersson, Stewart and Zidani [5] uses the Whitney Extension Theorem to formulate a conceptual model of how imperfectly fitting patches might be perturbed to form a topological complex which is the boundary of a non-empty compact element of $\mathcal{R}(\mathbb{R}^3)$. Furthermore, the proposed process extends the patches under Lipschitz mappings so that the resulting element of $\mathcal{R}(\mathbb{R}^3)$ can be shown to lie within rigorous error bounds of the given geometric input data. Our initial results on ambient isotopic approximations of 2-manifolds have followed the prevailing simplification of considering only those manifolds without boundaries [2, 28, 29], but our recent results have been for the more technically challenging cases of 2-manifolds with boundaries [1]. Our team is also completing work on spline intersections with multiple roots [23], to improve the rather loose error bounds known to-date.

Interestingly, the interval solids were not initially intended as a means to integrate issues of topological equivalence and approximations in intersection algorithms. Yet it is a hallmark of our project that these concepts are merging, as discussed above. Note, further, that the intervals include both approximation errors from truncation of numerical processes within intersection algorithms as well as the approximations that arise by using a finite set of floating point numbers in computation as an approximation of the reals. How floating point approximations effect error bounds for intersection computations is another important issue this project considers. Attention has focused upon the impact of floating point arithmetic on polynomial computations near multiple roots [16]. This is an important issue because the intersection algorithms have to search for roots of the system of polynomial equations representing the intersecting surfaces and exact arithmetic computations have not been shown to be practical.

5. Conclusions and future work

Topology and computer science are finding common interest in the emerging area of computational topology. Various branches of pure topology (point-set topology, differential topology, low-dimensional topology, ...) can make important contributions to establishing the appropriate theoretical foundations. A fundamentally new perspective arises from the role that computational approximations should play in the reformulation of central topological concepts. The I-TANGO project is a research effort concentrating upon these issues specifically with respect to surface intersections within $\mathbb{R}^3$. Considerable progress has already been made, but many questions also remain open, as is summarized in this article.

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